Combustion Research Facility News

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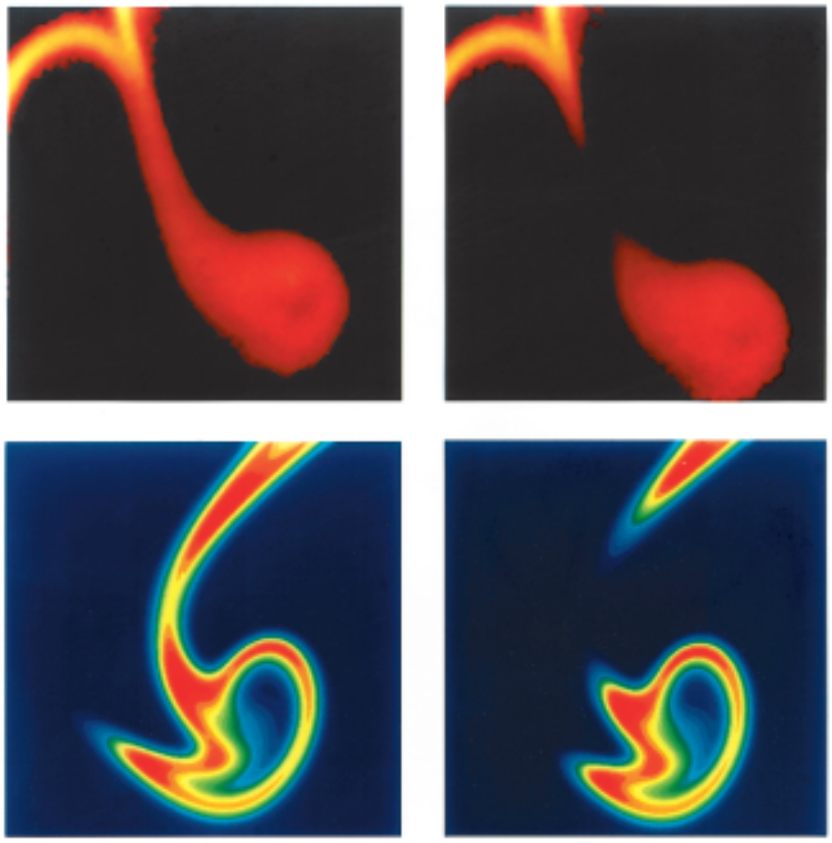
Understanding and modeling pocket formation in turbulent flames

Jacqueline Chen, Tarek Echekki, Wolfgang Kollmann and Phillip Paul have been studying flame-flame interactions in turbulent combustion, phenomena that can result in the formation of unburnt pockets of reactants. Models of turbulent combustion often are based on understanding of isolated laminar flames, yet in practical turbulent combustion environments, ensembles of flames continuously interact with one another and, through their interactions, influence the global properties of the flame. Models that account for these interactions under turbulent conditions do not currently exist.

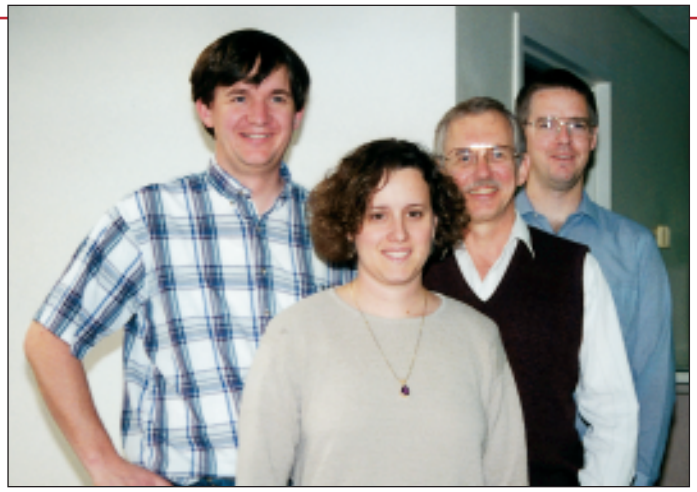
Direct numerical simulation (DNS), planar laser-induced fluorescence (PLIF) imaging , and theory are used to investigate the mechanism of unburnt pocket formation in an unsteady premixed hydrocarbon flame/vortex interaction, a building-block flow for turbulent combustion. Results from DNS and experiments show that pocket formation involves three distinct stages: (1) flame channel closing involving head-on quenching of flames, (2) cusp recovery, and (3) pocket burnout. The first two stages are revealed in images of formaldehyde shown in the figure, a combustion intermediate found in the oxidation of hydrocarbon fuels, as obtained both from computation and experiment.

The images clearly show that pocket formation is a highly transient event resulting in topological changes to the flame front. In both the computation and experiment the channel closes off in less than one-tenth of a flame time. Results from DNS show that the acceleration of the flame prior to channel closing is attributed to a change in the balance between reaction and transport within the flame and to changes in the profiles of the various scalars. As the primary fuel consumption layers disappear by mutual annihilation, flame chemistry shifts from reactions characterizing the hydrocarbon/air system to reactions favoring the hydrogen/air system. One outcome of the chemical changes is a temporary enhancement in the radical pool. This in turn precipitates the acceleration of the flame during the final stages of channel closing.

It is also found that flame stretch, the fractional change in the flame surface area, becomes singular as the flames merge. The source term associated with stretch in the flame surface density function equation for turbulent premixed combustion is traditionally modeled as a separate term. In the present work, theory and DNS show that the normal restoration and the turbulent dissipation portions of the source term become singular. However, their singularities are balanced; hence, their sum, and not the individual terms, need to be modeled. Detailed modeling of the source terms in this equation is a topic Jacqueline and Wolfgang are investigating.



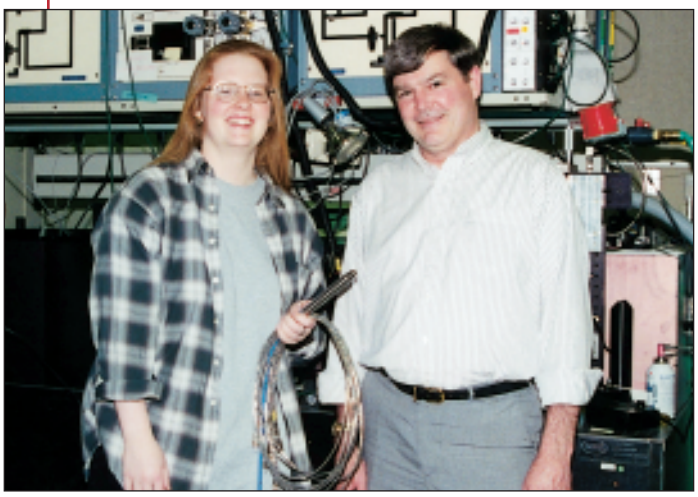
Formaldehyde images showing unsteady flame/vortex interaction leading to pocket formation in a premixed methanol/air flame (PLIF images, top row) and in a premixed methane/air flame (DNS images, bottom row).



Melissa Lunden, a post-doctoral fellow from California Institute of Technology, recently completed her assignment with Chris Shaddix (back right), Jimmy Ross, Allen Robinson, and Robert Hurt (Brown University), under the direction of Don Hardesty (center back right), in the coal combustion laboratory. Several projects that involved characterizing the oxidation kinetics of coal and biomass chars were completed. She also worked with Larry Baxter (left) and Steve Buckley to measure and predict fine particulate emissions from biomass combustion for use in a project to remediate the radioactive contamination in Belarus from the Chernobyl power plant incident.

Engine combustion CRADA reviews held

The Engine Combustion Department recently participated in several CRADA (cooperative research and development agreements) reviews. The reviews covered work with Cummins, Caterpillar, and Detroit Diesel focusing on diesel combustion issues in the heavy-duty class of engines utilizing both conventional as well as alternative diesel fuels. Reviews with Chrysler, Ford, and General Motors were held to discuss progress on CRADAs related to combustion issues for automobile engines. These projects investigate port-fuel injection and direct-injection (spark-ignition and compression-ignition) engines.



Janeen Ault, a graduate student from Imperial College, London, has been assisting Pete Witze for the past year in studying flame kernel development in spark ignition engines using a Fiber Optic Spark Plug probe, which she is holding. In the fall, Janeen will continue her studies at the University of Wisconsin, Madison, as a research assistant in the Solar Energy Lab.

Construction was completed on the CRF Phase II Laboratory Building in May, and Principal Investigators are now in the process of equipment installation and checkout. Several of the labs are expected to be operational this summer, with the balance coming on line in early 1999. The Alternative Fuels lab (shown: Sal Birtola; Chuck Mueller, PI; Lloyd Claytor; and Jim Boehmke) is among the first to become operational. Roger Farrow's Diagnostics lab and Phil Paul's Advanced Imaging lab are also nearing completion.

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Cluster-dissociation provides new insights into energy transfer models

Recent studies performed in the chemical dynamics laboratory on the dissociation of van der Waals clusters demonstrate a method for measuring the probability distribution for vibrational to translational energy transfer (V-T) in large polyatomic systems. Thomas Lorenz and David Chandler, in collaboration with Laurie Yoder and John Barker of the University of Michigan, have acquired ion images of pyrazine recoil distributions resulting from the unimolecular dissociation of pyrazine-argon van der Waals clusters. The cluster fragmentation is the result of an internal V-T energy transfer process.

The vibrational predissociation of a van der Waals cluster is a half-collision analog of a full bimolecular collision between a vibrationally excited molecule and its collision partner. Figure 1 illustrates how a "well-defined" collision can be prepared and the ensuing dynamics probed directly. Pyrazine-Ar complexes produced in a seeded molecular beam are excited from the ground electronic state to the first excited singlet state, designated S_0 and S_1, respectively. The excited pyrazine rapidly converts to an excited triplet state having about 0.5eV of vibrational energy.

At this point the complex has a well-defined vibrational energy distribution and collision orientation. A portion of this vibrational energy is transferred to the argon atom causing fragmentation of the complex. The recoiling pyrazine fragment retains its triplet character long enough to be photoionized by a second laser and imaged onto a 2-dimensional position-sensitive detector.

The top of Figure 2 shows intensity distributions for pyrazine ions originating from pyrazine entrained in the molecular beam and pyrazine recoiling from fragmenting clusters. The spread in positions reflects the spread in velocities of the pyrazine molecules. It is clear that the cluster fragments have a greater velocity spread owing to the additional kick received in the vibrational energy transferred out of the triplet state. The graph below shows positional data taken from the images and transformed into a set of radial distributions. An analysis of the radial distributions will give the probability distribution for V-T energy transfer for this process.

Collisional energy transfer processes play a crucial role in many chemical reactions. Intermolecular collisions provide a means of exchanging energy between collision partners allowing for chemical activation of reactants or for the relaxation of energetic products, ultimately to thermal equilibrium. The present study provides a direct measure of the energy transfer between collision partners under single collision conditions and well-defined energy constraints. Other experiments typically give measured values that are indirect or that are averaged over many collisions and relative collision energies.

The efficiencies for transferring energy between vibrational, rotational and translational degrees of freedom can vary dramatically from system to system. V-T transfer is typically an inefficient process and normally requires a large number of successive collisions to build up enough energy exchange that can be accurately measured. The ion imaging technique is sensitive to single particles and relatively low velocities, making it especially suitable for studying these types of low efficiency transfer processes.

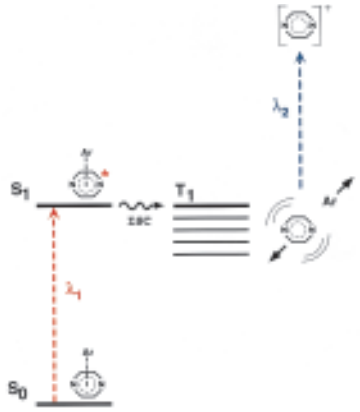


Figure 1. Illustration of experimental methodology. Vibrationally hot cluster complexes are prepared via excitation to the S_1 state followed by intersystem crossing to the T_1 triplet state. Cluster fragmentation occurs in the T_1 state. A short time later (20ns) the recoiling pyrazine is photoionized and imaged.

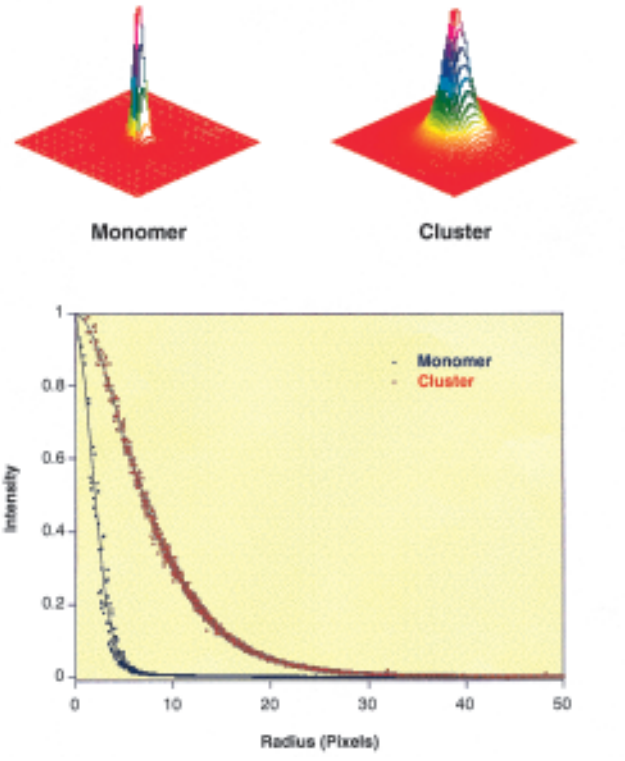


Figure 2. (Top): Ion Images of pyrazine monomers entrained in the molecular beam and nascent pyrazine fragments from cluster fragmentation, designated monomer and cluster, respectively. (Bottom): Data from images which has been transformed to radial distributions. The increased spread in the radial distribution for the cluster fragments provides a measure of the V-T energy transfer process.

Fiber-optic spark plug probe revisited

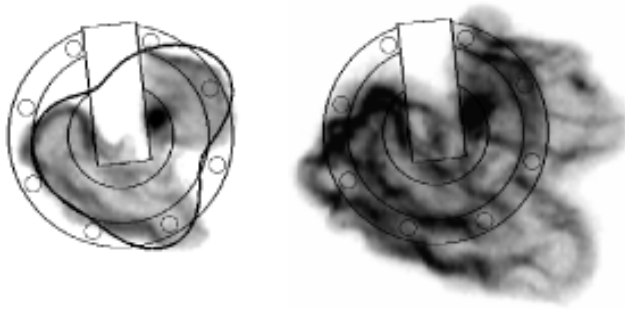
Cycle-by-cycle variations in the combustion process of premixed-charge spark-ignition engines are a common problem that affects driveability and performance. A major cause is variations in the growth rate and location of the early flame kernel. Responding to a request from industry, Janeen Ault and Pete Witze have taken a new look at analysis procedures for data obtained with the fiber-optic spark plug (FOSP) that Pete first developed ten years ago.

The probe consists of a standard spark plug with eight optical fibers installed in a ring at the base of the threaded region of the plug. The fibers collect light emitted from the flame as it crosses the field of view of the fibers, and transmit the light to photomultiplier tubes. The time from ignition until detection of the flame is used to compute the average flame velocity in the direction of each fiber relative to the spark location. These eight measurements are then input into a model to calculate the convective velocity V_c of the flow, and the expansion speed S_g of the flame kernel.

A common problem encountered by users of the probe has been uncertainty in how to reliably identify flame arrival from the luminosity signals, particularly for light load and lean operating conditions and when there is interference from the spark. To investigate this, Janeen and Pete obtained visible-emission images of the developing flame simultaneously with the FOSP measurements. By comparing the flame images with the analog photomultiplier-tube signals, they were able to develop a reliable and automatic procedure for determining flame arrival. In addition, sequential images of the developing flame were taken to evaluate the assumptions of the model for calculating V_c and S_g, as well as to study the evolution of the flame shape with time.

As an alternative to using a costly, fast-framing-rate intensified camera, they used a single, intensified CCD camera that they synchronized with the engine cycle. This permitted the acquisition of a flame image at the end of one video field and the beginning of the next, similar to a technique used for PIV (particle image velocimetry). The image on the second field includes a double exposure of the first field, but because the flame typically grows faster that it moves, this is not a problem.

An example of processed flame images taken in this manner is shown in the figure. The flame image on the left was taken at 4 crank-angle-degrees (CAD) after ignition, while the image on the right was taken at 7 CAD after ignition. Overlaid on the earlier flame image is a cubic-spline contour determined from the flame arrival times obtained with the FOSP, which does a good job at matching the shape of the actual flame. Double images like these not only aid in interpretation of the FOSP signals, but allow us to calculate V_c and S_g directly from the images for comparison with the values obtained solely by the FOSP.



Sequential images of flame development in an SI engine run lean at 300 rpm. The flame image on the left was taken 4 degrees after ignition, and the image on the right was obtained 3 degrees later.

NOTICE

The Sandia Combustion Research 1998 Technical Review will be available on the CRF Website, www.ca.sandia.gov/CRF/, on or about July 1.

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